

# **Supporting Information for**

## **Facile Electron Transfer to CO<sub>2</sub> throughout Adsorption at the Metal | Solution Interface**

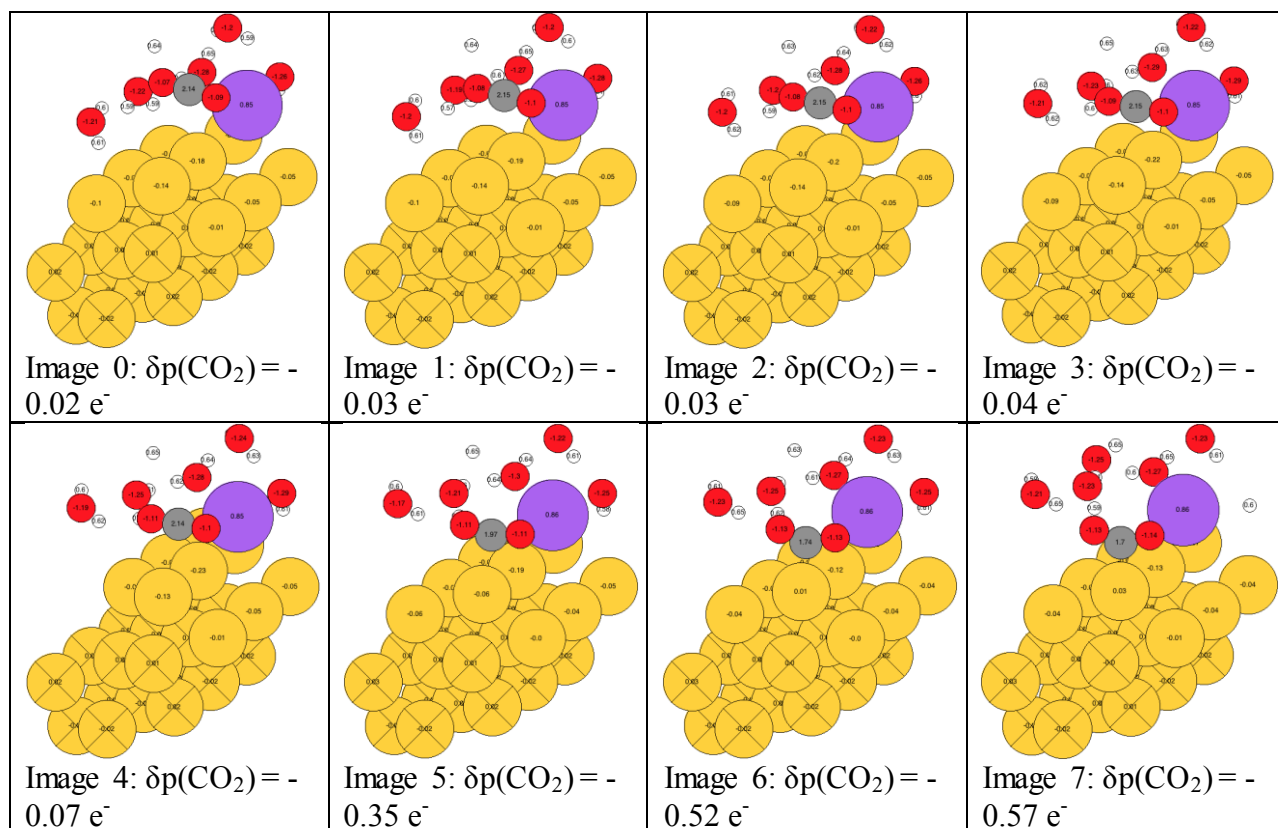
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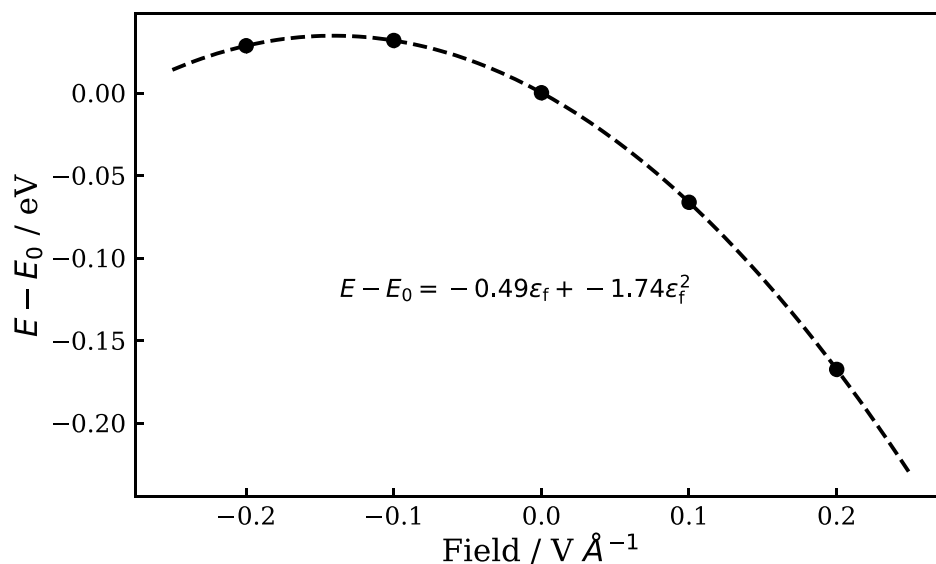
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**Figure S1:** Calculated Bader charges on CO<sub>2</sub> for structures from Figures 1 and 3 in the main text.



**Figure S2:** Electric field effect on CO<sub>2</sub> adsorption energy. The induced dipole moment is  $-0.49 e\text{\AA}$ .

**Table S1. Tabulated Figure 1 Data.**  $E_{\text{ref}}$  represents the reference energy of the system when  $\text{CO}_2$  is very far from the surface. We represent this by adding the energy of gas phase  $\text{CO}_2$  to the energy of an optimized clean slab and solvent layer, where:  $E_{\text{clean}} = -141.41459015$  eV  $E_{\text{CO}_2}(\text{g}) = -22.26223813$  eV. All structures and energies for Figures 1-4 are available for download at <https://www.catalysis-hub.org/publications/GauthierFacile2019>.

Adiabatic Curve		
x-axis (image #)	Raw Energies	y-axis ( $E - E_{\text{ref}}$ eV)
0	-163.7475105	-0.07068222
1	-163.71015173	-0.03332345
2	-163.62857459	0.04825369
3	-163.516071	0.16075728
4	-163.39262956	0.28419872
5	-163.26518023	0.41164805
6	-163.37250524	0.30432304
7	-163.39387461	0.28295367

**Table S2. Tabulated Data of Figure 3 analogous to Table S1.** All structures and energies for Figures 1-4 are available at <https://www.catalysis-hub.org/publications/GauthierFacile2019>.<sup>1</sup>

Diabatic Curve (Linear)		
x-axis (image #)	Raw Energies	y-axis ( $E - E_{\text{ref}}$ eV)
0	-163.74751045	-0.07068217
1	-163.70984392	-0.03301564
2	-163.62736444	0.04946384
3	-163.50996462	0.16686366
4	-163.3691322	0.30769608
5	-162.94906371	0.72776457
6	-161.86091396	1.81591432
7	-161.62124948	2.0555788

Diabatic Curve (Bent)		
x-axis (image #)	Raw Energies	y-axis ( $E - E_{\text{ref}}$ eV)
0	-162.36710234	1.30972594

1	-162.38279712	1.29403116
2	-162.39349499	1.28333329
3	-162.42470949	1.25211879
4	-162.53774454	1.13908374
5	-162.99744176	0.67938652
6	-163.35836356	0.31846472
7	-163.39387461	0.28295367